L2

(FILE 'HOME' ENTERED AT 08:58:17 ON 28 DEC 2007)

FILE 'REGISTRY' ENTERED AT 08:58:24 ON 28 DEC 2007

L1 995518 S NCSC2/ES

STRUCTURE UPLOADED

L3 12 S L2 SAM SUB=L1

L4 217 S L2 SSS FULL SUB=L1

FILE 'CAPLUS' ENTERED AT 08:59:36 ON 28 DEC 2007

L5 9 S L4

FILE 'REGISTRY' ENTERED AT 08:59:41 ON 28 DEC 2007

SAV TEM L4 BRD555664/A

FILE 'CAPLUS' ENTERED AT 09:00:12 ON 28 DEC 2007

1 S US200!-555664/APPS

L7 1 S L5 AND L6

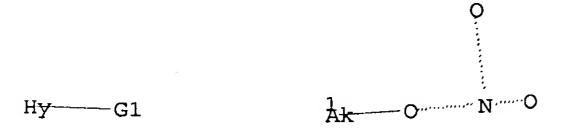
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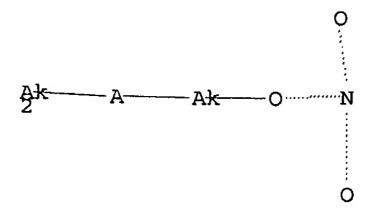
FILE 'REGISTRY' ENTERED AT 09:00:40 ON 28 DEC 2007

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L2 HAS NO ANSWERS

L2 STR

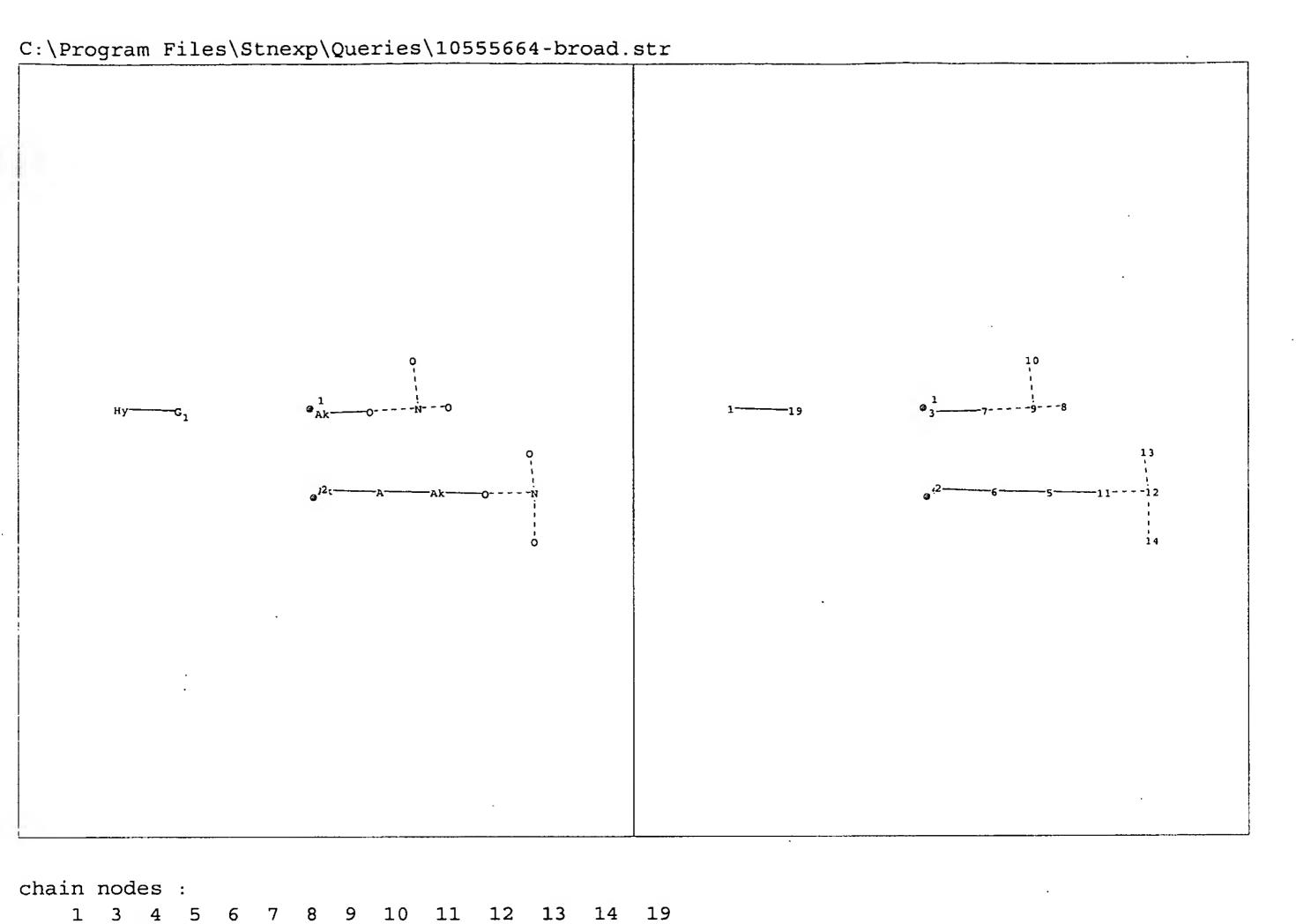




G1 [@1], [@2]

Structure attributes must be viewed using STN Express query preparation.

=>



11-12

11-12

12-13

12-13

12-14

12-14

G1:[*1],[*2]

chain bonds :

exact/norm bonds :

1-19 3-7 4-6

Connectivity :

3:2 E exact RC ring/chain 4:2 E exact RC ring/chain 5:2 E exact RC ring/chain Match level:

8-9 9-10

8 - 9

9-10

1:Atom 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 19:CLASS

Generic attributes :

1:

Saturation : Unsaturated Number of Carbon Atoms : less than 7 Number of Hetero Atoms : 2 or more Type of Ring System : Monocyclic

1-19 3-7 4-6 5-6 5-11 7-9

5-6

5-11

7-9

Element Count :

Node 1: Limited

S,S1

N,N1

C,C3

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COPYRIGHT 2007 ACS on STN
                    CAPLUS
     ANSWER 1 OF 1
L7
     2005:1192912
                   CAPLUS
AN
     143:460140
DN
     Preparation of thiazole derivatives as nitric oxide donors for treating
TI
     inflammatory bowel diseases
     Assaf, Peter
IN
     Renopharm Ltd., Israel
PA
     PCT Int. Appl., 126 pp., which
SO
     CODEN: PIXXD2
DT
     Patent
     English
LA
FAN.CNT 1
                                 DATE
                                             APPLICATION NO.
                                                                     DATE
     PATENT NO.
                         KIND
                                                                     20050505
                          A2
                                 20051110
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PI
     WO 2005105065
                                 20051215
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     WO 2005-IL481
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                                 20050505
OS
     MARPAT 143:460140
GI
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Use of a novel class of NO-donating compds. of formula I [A = alkenyl, alkoxy, alkyl, aryl, NH, diazo, disulfide, etc.; X = alkyl, alkoxy, aryl, aryloxy, CN, cycloalkyl, heteroaryl, etc.; B = alkylene, heteroalkylene, etc.; Y = NO-releasing group; Z = H, alkyl, NH2, cycloalkyl, aryl, halo, OH, alkoxy, etc.], designed such that when NO is released from the compound a residue which is a naturally occurring metabolite is formed, in the treatment of inflammatory bowel diseases is disclosed. Thus, II was prepared, and had Δ OD460 value of 12.75 in MPO activity tests in colon tissues from colitis-induced rats.

10555664

2 of 18

ANSWER 1 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN 2005:547257 CAPLUS Full-text AN DN 143:77866 Preparation of nitrate esters having a \$\beta\$- or y-sulfur atom for TI protection of cells/tissues from oxidative damage. Thatcher, Gregory R. j.; Bennett, Brian M.; Reynolds, James N.; Boegman, IN Roland J.; Jhamandas, Khem USA PA U.S. Pat. Appl. Publ., 83 pp., Cont.-in-part of U.S. Ser. No. 147,808. SO CODEN: USXXCO DT Patent English LA FAN. CNT 6 APPLICATION NO. DATE DATE KIND PATENT NO. ----...... US 2005137191 20050623 US 2004-943264 20040917 Al 19980915 US 1996-658145 19960604 US 5807847 A US 1997-867856 19970603 19990316 US 5883122 US 1999-267379 19990315 US 6310052 ₿1 20011030 19991229 US 7115661 20061003 US 1999-473713 20050330 EP 2004-28372 20001227 EP 1518553 A2 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR 20020520 US 2002177622 Al 20021128 US 2002-147808 US 6916835 20050712 20050916 AU 2005284573 A1 20060323 AU 2005-284573 20050916 20060323 CA 2005-2580627 CA 2580627 Al 20050916 WO 2006029532 Al 20060323 WO 2005-CA1417 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ,

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YXCR3R4 (CR17R18) n (CR1R2) moNo2 [m, n = 0-10; R3, R4, R17 = H, nitrate, A; R1 = H, A; A = (substituted) (unsatd.) (cyclic) aliphatyl; R1R3, R4R17 = aliphatyl linkage; R2, R18 = H, A, XY; X = F, Cl, Br, Cl, NO2, CH2, CF2, O, NH, NMe, cyano, NHOH, N3, S, SCN, SO, SO2, etc.; Y = null, F, Cl, Br, Cl, Me, CF2H, CF3, OH, NH2, S, SCN, SH, etc.; with provisos], were prepared Thus,

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854925-93-2 CAPLUS

2,5-Thiazoledimethanol, 4-methyl-α2-(trifluoromethyl)-, dinitrate (ester) (9CI) (CA INDEX NAME)

854925-94-3 CAPLUS

2,5-Thiazolediethanol, 4-methyl-β2-3-thienyl-, dinitrate (ester) (9CI) (CA INDEX NAME)

854925-95-4 CAPLUS

INDEX NAME)

2,5-Thiazoledimethanol, α2,4-dimethyl-, dinitrate (ester) (9CI) (CA

854925-96-5 CAPLUS

5-Thiazoleethanol, 4-methyl-2-[2,2,2-trifluoro-1-(nitrooxy)ethyl]-, nitrate (ester) (9CI) (CA INDEX NAME)

[O2NOCH2CH(ONO2)CH2S]2 (prepared via the corresponding Bunte salt) at 200 µmol/kg s.c. gave virtually complete protection against 6-OHDA killing of dopaminergic neurons in rats.

854925-90-9P 854925-91-0P 854925-92-1P 954325-93-2P 954925-94-3P 854925-95-4P 854925-96-5P 854925-98-7P 854925-99-5P 554926-00-4P 554926-02-6P 654926 01-7F 854926 06-0P 854926-07-1P 854926-03-CP 954918 09-3P 954926-10-6F 954926-31 7P 954926-12-aP 954925-13-9P 354925-34-9P 884926-15-1P 884936-17-3P 854926-18-4P 854926-26-4P 954926-28-6P 854925-39-6P 854926-31-19 854926-32-29 854926-33-39

554926-34-4P \$54926-37-7P 854926-28-8E

854926-41-39 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(claimed compound; preparation of nitrate esters having $\beta\text{-}$ or y-sulfur atom for protection of cells/tissues from oxidative damage)

854925-90-9 CAPLUS 5-Thiazoleethanol, 4-methyl-2-[1-(nitrooxy)-1-(3-thienyl)ethyl]-, nitrate

(ester) (9CI) (CA INDEX NAME)

(CA INDEX NAME)

854925-91-0 CAPLUS 5-Thiazoleethanol, 4-methyl-2-[1-(nitrooxy)ethyl]-, nitrate (ester) (9CI) CN

854925-92-1 CAPLUS 2,5-Thiazolediethanol, 4-methyl-, dinitrate (ester) (9CI) (CA INDEX NAME)

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Ethanone, 1-[4-methyl-5-[(nitrooxy)methyl]-2-thiazolyl]- (CA INDEX NAME)

854925-99-8 CAPLUS

5-Thiazoleethanol, 4-methyl-2-[2,2,2-trifluoro-1-(3-thienyl)ethyl]-, nitrate (ester) (9CI) (CA INDEX NAME)

854926-00-4 CAPLUS

Ethanone, 2,2,2-trifluoro-1-{4-methy1-5-[2-(nitrooxy)ethy1}-2-thiazoly1]-(CA INDEX NAME)

854926-02-6 CAPLUS

Methanone, (4,5-dimethyl-2-thiazolyl)[4-methyl-5-[2-(nitrooxy)ethyl]-2thiazolyl) - (CA INDEX NAME)

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854926-03-7 CAPLUS

5-Thiazoleethanol, 2-(methoxymethyl)-4-methyl-, nitrate (ester) (9CI) (CA

854926-06-0 CAPLUS

2-Thiazolemethanol, 5-(methoxymethyl)-u,4-dimethyl-, nitrate (ester) (9CI) (CA INDEX NAME)

854926-07-1 CAPLUS

2-Thiazolemethanol, a,4,5-trimethyl-, nitrate (ester) (9CI) (CA INDEX NAME)

854926-08-2 CAPLUS

5-Thiazoleethanol, 4-methyl-2-[2-methyl-1-(nitrooxy)propyl]-, nitrate (ester) (9CI) (CA INDEX NAME)

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854926-14-0 CAPLUS

5-Thiazolemethanol, 4-methyl-2-[4-(trifluoromethyl)phenyl]-, nitrate (ester) (9CI) (CA INDEX NAME)

854926-15-1 CAPLUS

5-Thiazoleethanol, 4-methyl-2-[4-(trifluoromethyl)phenyl)-, nitrate (ester) (9CI) (CA INDEX NAME)

954926-17-3 CAPLUS

5-Thiacoleethanol, 4-(4-chlorophenyl)-2-phenyl-, nitrate (ester) (9CI) CN (CA INDEX NAME)

854926-18-4 CAPLUS

5-Thiazolemethanol, 2-(4-chlorophenyl)-4-methyl-, nitrate (ester) (9CI) (CA INDEX NAME)

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6 of 18

854926-09-3 CAPLUS 5-Thiazoleethanol, 4-methyl-2-phenyl-, nitrate (ester) (9CI) (CA INDEX NAME)

854926-10-6 CAPLUS

5-Thiazoleethanol, 2,4-dimethyl-, nitrate (ester) (9CI) (CA INDEX NAME)

RN 854926-11-7 CAPLUS

5-Thiazoleethanol, 4-methyl-2-(2,2,2-trifluoro-1-hydroxyethyl)-, nitrate (ester) (9CI) (CA INDEX NAME)

854926-12-8 CAPLUS

5-Thiazoleethanol, 2-(4-chlorophenyl)-4-methyl-, nitrate (ester) (9CI) (CA INDEX NAME)

854926-13-9 CAPLUS

5-Thiazolemethanol, 4-methyl-2-phenyl-, nitrate (ester) (9CI) (CA INDEX CN

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RN 854926-26-4 CAPLUS

2-Thiazoleethanol, nitrate (ester) (9CI) (CA INDEX NAME)

RN 854926-28-6 CAPLUS

CN 2-Thiazolemethanol, α-methyl-, nitrate (ester) (9CI) (CA INDEX

RN 854926-30-0 CAPLUS

CN 2-Thiazoleethanol, α-methyl-, nitrate (ester) (9CI) (CA INDEX NAME)

RN 854926-31-1 CAPLUS

CN 5-Thiazoleethanol, α -butyl-, nitrate (ester) (9CI) (CA INDEX NAME)

RN 854926-32-2 CAPLUS

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2-Thiazolemethanol, α -(1,1-dimethylethyl)-, nitrate (ester) (9CI) (CA INDEX NAME)

854926-33-3 CAPLUS

2-Thiazolemethanol, α-pentyl-, nitrate (ester) (9CI) (CA INDEX NAME)

854926-34-4 CAPLUS

CN 2-Thiazoleethanol, α -butyl-, nitrate (ester) (9CI) (CA INDEX NAME)

RN 854926-37-7 CAPLUS

5-Thiazoleethanol, α-butyl-4-methyl-, nitrate (ester) (9CI) (CA

854926-38-8 CAPLUS

5-Thiazoleethanol, 4-(trifluoromethyl)-, nitrate (ester) (9CI) (CA INDEX NAME)

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ANSWER 2 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

2001:792327 CAPLUS Full-text AN 135:339273

TI Nitrate esters, their preparation and use for treatment of neurological conditions

Thatcher, Gregory R. J.; Bennett, Brian M.; Reynolds, James N.; Boegman, IN

Roland J.; Jhamandas, Khem

Queen's University At Kingston, Can. U.S., 57 pp., Cont.-in-part of U.S. 5,883,122.

CODEN: USXXAM

Patent

LA	Eng	glish																
FAN.	CNT	6																
								APPLICATION NO.										
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ΡΙ	US 6310052				B1 20011030			US 1999-267379			19990315							
	US 5807847 US 5883122				A 19980915			US 1999-267379 US 1996-658145			19960604							
	O3 3003122				W TYYYUJIO			03 1331-001030					13310003					
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GI	- urti																	

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10 of 18

854926-41-3 CAPLUS

5-Thiazolemethanol, a-methyl-4-(trifluoromethyl)-, nitrate (ester) (9CI) (CA INDEX NAME)

IT 252558-49-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(preparation of nitrate esters having β - or γ -sulfur atom for

protection of cells/tissues from oxidative damage) 252568-49-3 CAPLUS

5-Thiazoleethanol, 4-methyl-, nitrate (ester) (9CI) (CA INDEX NAME)

IT 854926-52-6

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

(Biological study); USES (Uses)

(preparation of nitrate esters having $\beta\text{-}$ or $\gamma\text{-sulfur atom for}$

protection of cells/tissues from oxidative damage)

854926-52-6 CAPLUS

2-Thiazoleethanol, 5-(methoxymethyl)-4-methyl-, nitrate (ester) (9CI) (CA INDEX NAME)

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Title compds. O2NO-E-F-G [E, F, G = organic radicals; F, G = unsubstituted, unsubstituted pyridyl; when E = alkyl, F, G = not both alkyl radicals bearing nitrate groups or an O linkage; I) were prepared Examples include 7 bioassays and 13 synthetic examples. E.g., 2',3'-dideoxy-3-thiocytosine was nitrated (Ac20, HNO3, -30°C, 10 min) gave II in 52% yield. Certain examples I were shown to activate guanylyl cyclase. The invention is useful for treatment of neurol. or cognitive conditions.

252568-49-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(nitrate esters, preparation, and use for treatment of neurol. conditions) 252568-49-3 CAPLUS

THERE ARE 95 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 95 ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 3 OF 8 CAPLUS COPYRIGHT 2007 ACS ON STN LB 2001:507519 CAPLUS Full-text

AN 135:92207 DN

Synthesis, methods and compositions of organic nitrates for mitigating TI pain

Thatcher, Gregory R. J.; Bennett, Brian M.; Reynolds, James N.; Jhamandas, IN

Khem Queen's University at Kingston, Can.

PCT Int. Appl., 114 pp. SQ

CODEN: PIXXD2

AU 200123351

DT Patent LA English

FAN. CNT 6

	PATENT NO.	KIND DATE	APPLICATION NO.	DATE
PI	WO 2001049275	A2 20010712	NO 2000-CA1523	20001227
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20010716 AU 2001-23351

20001227

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10555664
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                                            EP 2004-28372
                                                                   20001227
        R: AT, BE, CH, DE, DK, ES, PR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, PI, CY, TR
                                20050331
     PT 1245625
                                            PT 2000-986925
                                                                   20001227
     ES 2233489
                          TЗ
                                20050616
                                            ES 2000-986925
                                                                   20001227
     HK 1050144
                          Al
                                20050708
                                            HK 2003-102415
                                                                   20030403
     US 2007066575
                                20070322
                                            US 2006-507995
                                                                   20060822
                          Al
PRAI US 1999-473713
                                19991229
                          A2
     EP 2000-986925
                          A3
                                20001227
     WO 2000-CA1523
                                20001227
     MARPAT 135:92207
     Methods and therapeutic compds. for treating pain, mitigating inflammation,
     effecting analgesia and/or effecting sedation in a subject are described. A
     subject is administered an effective amount of a therapeutic compound, e.g. 4-
     methylthiazole-5-Et nitrate (I), which is a nitrate ester. I shows a mean of
     54.21 s at 10 mg/kg in scoplamine-impaired learning assay. Novel
     pharmaceutical compns, are also described.
    25400 Feb. 49 349
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (synthesis, methods and compns. of organic nitrates for mitigating pain)
    252568-49-3 CAPLUS
    5-Thiazoleethanol, 4-methyl-, nitrate (ester) (9CI) (CA INDEX NAME)
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CH2- 0- NO2

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THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT 43
             ALL CITATIONS AVAILABLE IN THE RE FORMAT
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ANSWER 4 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

2000:666584 CAPLUS Full-text AN

133:232855 DN

ΤI Nitrate esters, their preparation, and their use for treatment of

neurological conditions

Thatcher, Gregory R. J.; Bennett, Brian M.; Reynolds, James N.; Boegman,

Roland J.; Jhamandas, Khem

Queen's University at Kingston, Can.

90 PCT Int. Appl., 115 pp.

CODEN: PIXXD2 DŤ

Patent

English FAN. CNT 6

PATENT NO. KIND DATE APPLICATION NO. DATE 20000921 WO 2000054756 A2 WO 2000-CA280 20000315

10555664

15 of 18

Treating nitrates, e.g. 2,4-(02N)2C6H3CH2CH2ONO2, with NaOH/EtOH gave alkenes, e.g., 2,4-(02N) 2C6H3CH:CH2.

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RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

5-Thiazoleethanol, 4-methyl-, nitrate (ester), compd. with

2,4,6-trinitrophenol (1:1) (9CI) (CA INDEX NAME)

CM

CRN 252569-49-3 CMF C6 H8 N2 Q3 S

CRN 88-89-1 CMF C6 H3 N3 O7

352539-49-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation of olefins from nitro esters) 252569-49-3 CAPLUS

5-Thiazoleethanol, 4-methyl-, nitrate (ester) (9CI) (CA INDEX NAME)

RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 6 OF 8 CAPLUS COPYRIGHT 2007 ACS ON STN 1965:488647 CAPLUS Full-text

10555664 14 of 18 WO 2000054756 20010125 W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MN, MX, NO, NZ, PL, PT, RO, RU, SD, SB, SG, SI, SK, SL, TJ, TM, TR, TT, T2, UA, UG, U2, VN, YU, ZA, ZN RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG US 6310052 Bı 20011030 US 1999-267379 20000315 CA 2364493 CA 2000-2364493 **A**1 20000921 EP 2000-910456 20000315 EP 1163029 A2 20011219 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO JP 2002539152 20021119 JP 2000-604832 20000315 20000315 AU 783036 AU 2000-32673 **B2** 20050915 MX 2001PA09246 20040326 MX 2001-PA9246 20010913 PRAI US 1999-267379 19990315 US 1996-658145 A2 19960604 US 1997-867856 19970603 A2 20000315 WO 2000-CA280 MARPAT 133:232855

Compds. and methods are described for mitigating neurodegeneration, effecting neuroprotection, and/or effecting cognition enhancement. Neurol. or cognitive conditions are treated by administering to a subject an effective amount of a therapeutic compound comprising a nitrate ester, or a pharmaceutically acceptable salt or ester thereof.

252569-43-3P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (nitrate esters, preparation, and use for treatment of neurol. conditions)

252568-49-3 CAPLUS 5-Thiazoleethanol, 4-methyl-, nitrate (ester) (9CI) (CA INDEX NAME)

ANSWER 5 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

1999:667043 CAPLUS Full-text AN

DN 132:35323

Nitroester chemistry, 21. Synthesis of olefins from nitroesters

Kochergin, P. M.; Blinova, L. S.; Karpov, G. A.; Mikhailova, I. S.;

Aleksandrova, E. V.; Korol, O. V. Center for Drug Chemistry-All-Russia Research Institute of Pharmaceutical

Chemistry, Moscow, Russia Pharmaceutical Chemistry Journal (Translation of Khimiko-

Farmatsevticheskii Zhurnal) (1999), 33(1), 41-44 CODEN: PCJOAU: ISSN: 0091-150X

Consultants Bureau

Journal

English

10555664 16 of 18

DN 63:88847

OREF 63:16327b-g

Thiazoles. XI. Synthesis and behavior of some new halogenated formylthiazoles

Silberg, A.; Frenkel, Z.

Univ. "Babes-Bolyai" Cluj, Rom.

Studia Universitatis Babes-Bolyai, Chemia (1965), 10(1), 27-31

Journal

CODEN: SUBCAB; ISSN: 1224-7154 Romanian cf. ibid., 9(2), 7-15 (1964); CA 61, 1606la. A new type of thiazolecarboxaldehyde was synthesized, in which the formyl group in position 4 of the thiazole mol. had a halogen as neighbor. Starting with 2-phenyl-4chloromethylthiazole (I), and boiling it with aqueous HNO3, 2-phenyl-4hydroxymethyl-5-chlorothiazole (II) was obtained. II (2 g.) was dissolved in 40 cc. hot acetic acid, adding while hot 0.8 g. Na2Cr2O7 -- 2H2O in 10 cc. hot acetic acid; a violent reaction took place and the solution turned green. The solution was heated for 1 hr. more on a water bath to yield 85% 2-phenyl-4formyl-5-chlorothiazole (III), m. 91-2*. III suffered no disproportionation in the Cannizzaro reaction, in contrast to 2-phenyl-4-formylthiazole. III (0.2 g.) and 0.2 g. malonic acid in a mixture of 0.8 cc. pyridine and 0.04 cc. piperidine was heated 1.5 hrs. on a hot water bath and boiled 15 min. to yield 2-phenyl-5-chloro-4-thiazoleacrylic acid (IV), m. 244-5° (EtOH). A similar reaction was obtained with 2-phenyl-4-formylthiazole. Boiling a solution of 0.2 g. III and 0.3 g. hydroxylamine-HCl in 1 cc. pyridine and 2 cc. absolute EtOH on a water bath gave 2-phenyl-4-formyl-5-chlorothiazole oxime (V), m. 185-6° (EtOH). A solution of 1.5 g. II in 7 cc. concentrated H2SO4 was chilled to -5° and 0.7 cc. fuming HNO3 (d. 1.51) added dropwise while stirring; the mixture was kept 45 min. at -5° and at room temperature to give quant. 2-(p-nitrophenyl)-4-hydroxymethyl-5- chlorothiazole nitric ester (VI), m, 92-3° (very little EtOH). The p-position of the nitro function was established by oxidation or hydrolysis of VI. By oxidation of VI as II, 2-(pnitrophenyl) -4-formyl-5-chlorothiazole (VII), m. 162-3°, was obtained in low yield. Treatment of VII as III gave 2-(p-nitrophenyl)-4-formyl-5chlorothiazole oxime (VIII), m. 2274. By dissolving 0.2 g. VI in min. 90-5% H2SO4, and heating for 15-20 min. at 60-70°, followed by pouring over ice, 2-(p-nitrophenyl)-4-hydroxymethyl-5-chlorothiazole (IX) was obtained in 70% yield, m. 180° (EtOH). IX was also obtained by nitration of I to 2-(pnitrophenyl)-4-chloromethyl-thiazole (X) followed by boiling 2.5 g. X in a mixture of 30 cc. HNO3 (d. 1.42) and 70 cc. H2O for 3 hrs., and cooling (70% yield). Oxidation of XI as of II gave VII in almost quant. yield. The ir spectra of the chlorothiazolecarboxaldehydes were very similar to those of the corresponding nonhalogenated aldehydes except for a slight shift of the vc=o towards higher values (1715 cm.-1). In the case of VII, the bands characteristic of the NO2 group appeared at the same values, 1525 and 1350 cm.-1, as in the case of 2-(p-nitrophenyl)-4- formylthiazole. 15 references.

4254-45-3P, 4-Thiazolemethanol, 5-chloro-2-(p-nitrophenyl)-,

nitrate (ester) RL: PREP (Preparation)

(preparation of)

4264-45-3 CAPLUS

4-Thiazolemethanol, 5-chloro-2-(p-nitrophenyl)-, nitrate (ester) (8CI)

10555664

17 of 18

L8 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2007 ACS ON STN

AN 1965:409582 CAPLUS Full-text

DN 63:9582

OREF 63:1663c-d

TI Stabilization of ascorbic acid in oral liquid formulations. III. Effect of vitamins

AU Das, Sudeb; Dutta, B. K.; Dutta, B. N.

CS Dey's Med. Stores (Mfg.) Pvt. Ltd., Calcutta, India

SO J. Proc. Inst. Chemists (1964), 36(5), 256-8

DT Journal LA English

The effect of different vitamins was investigated on the kinetics of AB degradation of vitamin C in 60:20:20 70% sorbitol solution-propylene glycolglycerol. To solns. of 100 mg. ascorbic acid/5 ml. base was added each of the following vitamins: 7.5 mg, thiamine-HCl; 7.5 mg, thiamine mononitrate; 7.5 mg. riboflavine; 7.5 mg. riboflavine 5'-phosphate; 7.5 mg. panthenol; 15 mg. Ca pantothenate; 75 mg. niacinamide; 7.5 mg. pyridoxine-HCl; 35 y cyanocobalamin; 1.5 mg. folic acid; 1.5 mg. menadione; 1500 I.U. vitamin A palmitate; 35 mg. inositol; and 185 y calciferol. The pH was adjusted to 3.4 and 50 ml, of each formulation stored in 4 oz. amber glass bottles at 70°. The potency of ascorbic acid was then determined at appropriate time intervals and the rate of degradation of ascorbic acid were calculated by the graphic modification of McLeod, et al. (CA 53, 649h) of Garrett's method (CA 50, 14183b) by application of the Arrhenius equation. Thiamine-HCl, panthenol, cyanocobalamin, folic acid, pyridoxine-HCl, vitamin A palmitate, riboflavine, inositol, and calciferol had no appreciable effect on the degradation of vitamin C. The degree of degradation of ascorbic acid was most marked with Ca

pantothenate, miacinamide, menadione, thiamine mononitrate, and riboflavine

5'-phosphate in decreasing order. IT 863004-05-7, Thiamine, nitrate (ester)

(ascorbic acid stability in oral liquid pharmaceutical containing)

RN 869004-05-7 CAPLUS

CN Thiazolium, 3-((4-amino-2-methyl-5-pyrimidinyl)methyl)-4-methyl-5-(2-(nitrooxy)ethyl)- (CA INDEX NAME)

L8 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1965:409581 CAPLUS Full-text

DN 63:9581

OREF 63:1663a-c

10555664 18 of 18

TI Stabilization of ascorbic acid in oral liquid formulations. II. Effect of pH and metallic ions

AU Das, Sudeb; Dutta, B. K.; Dutta, B. N.

CS Dey's Med. Stores (Mfg.) Pvt. Ltd., Calcutta, India

SO J. Proc. Inst. Chemists (1964), 36(5), 252-5

DT Journal

English The effect was investigated of pH and different metallic ions on the stabilization of ascorbic acid in the base 60:20:20 70% sorbitol solutionpropylene glycol-glycerol. To 20 mg. ascorbic acid/ml. base was added each of the following metallic salts (to a final concentration of 0.1%): CuSO4; CoCl2; Ca gluconate; FesO4; MgSO4; MnSO4; Na glycerophosphate; K glycerophosphate. The pH of each formulation was adjusted to 3.5 and 50 ml. of each formulation was stored at 70° in amber glass bottles. The potency of ascorbic acid was then determined at appropriate intervals by titration with iodine solution and rates of degradation calculated The maximum deleterious effect was produced by Cu++, followed by Fe++, K+, and Mg++; Na+, Co++, and Ca++ had little effect while Mn++ was practically without effect. The stability of ascorbic acid was determined in the base 60:20:20 70% sorbitol-propylene glycol-glycerol at pH's 2.11, 2.90, 3.74, 4.41, and 5.59 at 70°. The degradation constant decreased with increases in pH. There was a sharp increase in the KO value when the pH was increased from 2.1 to 3.75, while the changes in KO in the range pH 3.75-4.41 were very small and after 4.41 fell to 0.1000 mg./5 ml./hr. at pH 5.59.

T 849004-05-7, Thiamine, nitrate (ester)
(ascorbic acid stability in oral liquid pharmaceutical containing)

RN 869004-05-7 CAPLUS

CN Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-4-methyl-5-[2-(nitrooxy)ethyl]- (CA INDEX NAME)

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